Short Course on Multilevel Methods for PDE-Constrained Optimization and Variational Inequalities

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Outline Short Course

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- Part 1: Multilevel methods for PDE-constrained optimization based on adaptive discretizations and reduced order models
- Part 2: Multilevel methods and reduced order models for the optimization with variational inequalities

Outline Part 1

- Problem setting and basic concept
- Adaptive multilevel methods for time-dependent PDE-constrained optimization with control constraints
- Implementation of the error control criteria by error estimators
- Extension to reduced order models with error estimation
- Numerical results

PD(A)E-constrained Optimization Problem

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PDE-constrained Optimization Problem (P):

$$\min_{y \in Y, u \in U} \; J(y,u) \quad \text{subject to} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

Y	State space,	$U_{ad} \subset U$	Convex, closed set,
U	Control space (Hilbert space),	$J : Y \times U \to \mathbb{R}$	Objective function,
		$C : Y \times U_{ad} \to \Lambda^*$	State equation.

Working assumptions:

- $C(y,u) = 0$ represents a (system of) PD(A)E('s) with initial and/or boundary conditions.
- For any $u \in U_{ad}$ the state equation $C(y,u) = 0$ has a unique solution $y = y(u) \in Y$.
- J, C are $\mathcal{C}^1$ and $C_y(y,u) \in \mathcal{L}(Y, \Lambda^*)$ has a bounded inverse.

Simple Example: Parabolic Optimal Control Problem with Control Constraints

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$$\min J(y,u) := \frac{1}{2}\|y(T)-y_d\|^2_{L^2(\Omega)} + \frac{1}{2}\|y-y_Q\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2((0,T)\times\partial\Omega)}$$

$$\begin{aligned}
\text{subject to} \quad & y_t - \Delta y = 0 && \text{in } Q := (0,T)\times\Omega,\\
& \partial_n y + y = u && \text{on } (0,T)\times\partial\Omega,\\
& y(0) = y_0 && \text{in } \Omega\\
& a \le u \le b
\end{aligned}$$

$\Omega \subset \mathbb{R}^2,\ T, \alpha > 0,$

$Y = W(0,T) = \{y \in L^2(0,T;H^1(\Omega)) \ : \ y_t \in L^2(0,T;(H^1)^*(\Omega))\},$

$U = L^2((0,T)\times\partial\Omega),$

$y_0 \in L^2(\Omega), \quad y_d \in L^\infty(\Omega), \quad y_Q \in L^\infty(Q),$

$a, b \in L^\infty((0,T)\times\partial\Omega), \quad a < b.$

Multilevel Method for (P)

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PDE-constrained Optimization Problem (P):

$$\min_{y \in Y, u \in U} \ J(y, u) \quad \text{subject to} \quad C(y, u) = 0, \quad u \in U_{ad}.$$

Adaptive multilevel solver for (P)

- uses a **hierarchy of adaptive (FE) approximations** of (P)
- approximates (FE) discretizations with **reduced order models**
- controls accuracy by **error estimators**
- converges globally and controls approximation errors

Hierarchy of Approximations

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Infinite-Dimensional Problem: "Truth"

PDE-constrained Optimization Problem (P):

$$\min_{y\in Y, u\in U} J(y,u) \quad \text{s. t.} \quad C(y,u)=0, \quad u\in U_{ad}.$$

Adaptive FE Discretization: "FE-Truth" We generate adaptive approximations

$$(\mathbf{P}_{h_k}) \quad \min_{y^{h_k}\in Y_{h_k}, u^{h_k}\in U_{h_k}} J^{h_k}(y^{h_k},u^{h_k}) \quad \text{s. t.} \quad C^{h_k}(y^{h_k},u^{h_k})=0, \quad u^{h_k}\in U_{ad}^{h_k}.$$

Later: Adaptive Reduced Order Model Approximation:

$$(\mathbf{P}^r_{h_k}) \quad \min_{y^{h_k,r}\in Y^r_{h_k}, u^{h_k,r}\in U^r_{h_k}} J^{h_k,r}(y^{h_k,r},u^{h_k,r}) \text{ s. t. } C^{h_k,r}(y^{h_k,r},u^{h_k,r})=0, u^{h_k,r}\in U_{ad}^{h_k,r}.$$

Challenges

Questions:

- When to proceed to a more accurate discretization?
- How to choose the next adaptive discretization?
- How to invoke reduced order models?

Related Work

- POD-based optimization: Hinze, Kunisch, Sachs, Tröltzsch, Volkwein,...
- Trust-region POD: Arian, Fahl, Sachs, Schu et al., OSPOD: Volkwein et al.
- Inexact function/constraint evaluations: Pironneau, Polak; Heinkenschloss, Ridzal, Vicente; Nocedal; S.U.; Griewank, Walther; Hintermüller; Tröltzsch.
- Recursive multilevel optimization methods: Gratton, Sartenaer, Toint
- A posteriori error estimators: Bank, Bartels, Becker, Carstensen, Debrabant, Lang, Funken, Hoppe, Rannacher, Siebert, Süli, Zienkiewicz, Zhu, ...
- A posteriori error estimators in optimal control:
  - Goal oriented: Becker, Rannacher; Becker, Kapp, Rannacher; Meidner, Vexler; Vexler, Wollner; Deckelnick, Günther, Hinze; Wollner; Hintermüller, Hoppe
  - Residual type: Li, Liu, Ma, Tang; Liu, Yan; Hintermüller, Hoppe, Iliash, Kieweg; Rösch, Siebert; S.U.
- Error control for ROMs: Canuto, Dahmen, Grepl, Gunzburger, Heinkenschloss, Hinze, Iapichino, Maday, Patera, Quarteroni, Rozza, Sorensen, Tröltzsch, Urban, deVore, Volkwein, Willcox,...

Outline

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- Problem setting and basic concept
- Adaptive multilevel methods for time-dependent PDE-constrained optimization with control constraints
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Optimization Methods:
Full Space Approach vs. Reduced Approach

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Full space approach:

Consider (P) as optimization problem in (y, u).

PDE-constrained Optimization Problem (P):

$$\min_{y \in Y, u \in U} J(y,u) \quad \text{s. t.} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

- Solves PDE and optimization problem at the same time
- Linearizes PDE-constraint in every optimization iteration
- Attractive in particular for stationary problems

Optimization Methods:
Full Space Approach vs. Reduced Approach

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Reduced approach:

Reduce (P) to an optimization problem in u.

Reduced Problem:

$$\min_{u \in U} \quad \widehat{J}(u) := J(y(u), u) \quad \text{s. t.} \quad u \in U_{ad},$$

where $y(u)$ is the unique PDE solution: $C(y(u), u) = 0$.

- Existing PDE solvers usable in a modular way
- Attractive in particular for time dependent problems

In this talk:

We concetrate on multilevel methods for the reduced approach.

Variants for the full space approach are also available (multilevel SQP methods).

Necessary Optimality Conditions

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PDE-constrained Optimization Problem (P):

$$\min_{y \in Y, u \in U} \quad J(y,u) \quad \text{s. t.} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

Lagrangian Function:

$$L(y,u,\lambda) = J(y,u) + \langle \lambda, C(y,u) \rangle_{\Lambda,\Lambda^*}$$

Necessary Optimality Conditions:

Assume that our assumptions on J, C hold. If $(\bar{y}, \bar{u})$ is local optimal solution of (P) then there exists a Lagrange multiplier (adjoint state) $\bar{\lambda} \in \Lambda$ with

$$\begin{aligned} C(\bar{y},\bar{u}) &= 0 && \text{(State equation)}, \\ L_y(\bar{y},\bar{u},\bar{\lambda}) = J_y(\bar{y},\bar{u}) + C_y^*(\bar{y},\bar{u})\bar{\lambda} &= 0 && \text{(Adjoint equation)} \\ \bar{u} \in U_{ad}, \quad (L_u(\bar{y},\bar{u},\bar{\lambda}), u - \bar{u})_{U^*,U} &\geq 0 \ \ \forall\, u \in U_{ad} && \text{(Stationarity)} \end{aligned}$$

Necessary Optimality Conditions

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Time-dependent PDE-Constrained Optimization

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For **time-dependent PDEs**

- solving the

  linearized PDE

  or the

  nonlinear PDE

  accurately on the discrete level (e.g. with Rosenbrock methods) has about the **same computational costs**

This motivates:

We consider a multilevel optimization method based on the reduced problem.

Reduced Optimization Problem

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Reduced Problem:

$$\min_{u \in U} \ \widehat{J}(u) := J(y(u), u) \quad \text{s. t.} \quad u \in U_{ad},$$

where $C(y(u), u) = 0$.
Differentiating the identity

$$\widehat{J}(u) = J(y(u), u) = J(y(u), u) + \langle \lambda, C(y(u), u) \rangle_{\Lambda, \Lambda^*} = L(y(u), u, \lambda)$$

we obtain the well known

Adjoint representation of the reduced derivative:

- Solve $C(y, u) = 0$ for y. $\rightsquigarrow \widehat{J}(u) = J(y, u)$
- Solve $L_y(y, u, \lambda) = 0$ for λ (Adjoint equation). $\rightsquigarrow \widehat{J}'(u) = L_u(y, u, \lambda)$

Hessian: $\widehat{J}''(u)s$ requires additional linearized state and adjoint solve.

Necessary Optimality Conditions Revisited

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PDE-constrained Optimization Problem (P):

$$\min_{y \in Y, u \in U} \quad J(y,u) \quad \text{s. t.} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

Lagrangian Function:

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Necessary Optimality Conditions:

Assume that our assumptions on J, C hold. If $(\bar{y}, \bar{u})$ is local optimal solution of (P) then there exists a Lagrange multiplier (adjoint state) $\bar{\lambda} \in \Lambda$ with

$$\begin{aligned} C(\bar{y},\bar{u}) &= 0 && \text{(State equation)}, \\ L_y(\bar{y},\bar{u},\bar{\lambda}) = J_y(\bar{y},\bar{u}) + C_y^*(\bar{y},\bar{u})\bar{\lambda} &= 0 && \text{(Adjoint equation)} \\ \bar{u} - P_{U_{ad}}(\bar{u} - \nabla_u L(\bar{y},\bar{u},\bar{\lambda})) &= 0 && \text{(Stationarity)} \end{aligned}$$

Necessary Optimality Conditions Revisited

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PDE-constrained Optimization Problem (P):

$$\min_{y \in Y, u \in U} \quad J(y,u) \quad \text{s. t.} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

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Assume that our assumptions on J, C hold. If $(\bar{y}, \bar{u})$ is local optimal solution of (P) then there exists a Lagrange multiplier (adjoint state) $\bar{\lambda} \in \Lambda$ with

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Example: Optimal Control of 2D Navier-Stokes Equations

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$$\min J(y,u) := \tfrac{1}{2}\|y - y_Q\|^2_{L^2(Q)} + \tfrac{\alpha}{2}\|u\|^2_{L^2((0,T)\times\Omega_c)}$$

$$\text{subject to} \quad \begin{aligned} y_t + y\cdot\nabla y - \nu\Delta y + \nabla p &= 1_{\Omega_c} u && \text{in } Q := (0,T)\times\Omega,\\ \operatorname{div} y &= 0 \\ y &= 0 && \text{on } (0,T)\times\partial\Omega,\\ y(0) &= y_0 && \text{in } \Omega \\ a \le u &\le b \end{aligned}$$

$\Omega_c \subset \Omega \subset \mathbb{R}^2,\ T, \alpha > 0,$

$V = \overline{\{v \in C_0^\infty(\Omega) : \operatorname{div} v = 0\}}^{H_0^1}$, $H = \overline{\{v \in C_0^\infty(\Omega) : \operatorname{div} v = 0\}}^{L^2}$,

$Y = W(0,T) = \{y \in L^2(0,T;V) : y_t \in L^2(0,T;V^*)\}$,

$U = L^2((0,T)\times\Omega_c)$,

$y_0 \in H, \quad y_Q \in W(0,T)$,

$a, b \in L^\infty((0,T)\times\Omega_c), \quad a < b.$

Example: Optimal Control of 2D Navier Stokes Equations

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Objective function: $J(y,u) := \frac{1}{2}\|y - y_Q\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2((0,T)\times\Omega_c)}$

State equation: $y \in Y = W(0,T), \quad C(y,u) = 0$ is given by

$$\langle y_t + y\cdot\nabla y - 1_{\Omega_c} u, v\rangle_{L^2(0,T;V^*),L^2(0,T;V)} + \nu(\nabla y, \nabla v)_{L^2} = 0 \quad \forall\, v \in L^2(0,T;V),$$
$$(y(0) - y_0, v_0)_{L^2} = 0 \quad \forall\, v_0 \in H.$$

Example: Optimal Control of 2D Navier Stokes Equations

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$$(y(0) - y_0, v_0)_{L^2} = 0 \quad \forall\, v_0 \in H.$$

Lagrangian: $\lambda = (w, w_0) \in \Lambda = L^2(0,T;V) \times H$

$$L(y,u,\lambda) = J(y,u) + \langle y_t + y \cdot \nabla y - 1_{\Omega_c} u, w \rangle_{L^2(0,T;V^*),L^2(0,T;V)} + \nu(\nabla y, \nabla w)_{L^2}$$
$$+ (y(0) - y_0, w_0)_{L^2}.$$

Example: Optimal Control of 2D Navier Stokes Equations

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Objective function: $J(y,u) := \frac{1}{2}\|y - y_Q\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2((0,T)\times\Omega_c)}$

State equation: $y \in Y = W(0,T), \quad C(y,u) = 0$ is given by

$$\langle y_t + y \cdot \nabla y - 1_{\Omega_c} u, v\rangle_{L^2(0,T;V^*),L^2(0,T;V)} + \nu(\nabla y, \nabla v)_{L^2} = 0 \quad \forall\, v \in L^2(0,T;V),$$
$$(y(0) - y_0, v_0)_{L^2} = 0 \quad \forall\, v_0 \in H.$$

Lagrangian: $\lambda = (w, w_0) \in \Lambda = L^2(0,T;V) \times H$

$$L(y,u,\lambda) = J(y,u) + \langle y_t + y \cdot \nabla y - 1_{\Omega_c} u, w\rangle_{L^2(0,T;V^*),L^2(0,T;V)} + \nu(\nabla y, \nabla w)_{L^2}$$
$$+ (y(0) - y_0, w_0)_{L^2}.$$

Adjoint equation: $L_y(y,u,\lambda) = 0$, $\lambda = (w, w_0) \in \Lambda$ is given by

$$(y - y_Q, v)_{L^2} + \langle v_t + v \cdot \nabla y + y \cdot \nabla v, w\rangle_{L^2(0,T;V^*),L^2(0,T;V)}$$
$$+\nu(\nabla v, \nabla w)_{L^2} + (v(0), w_0)_{L^2} = 0 \quad \forall\, v \in W(0,T).$$

Reduced derivative: $\widehat{J}'(u) = L_u(y,u,\lambda) = \alpha u - 1_{\Omega_c} w.$

Basic Trust Region Method 1

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$$\min_{u \in U} \ \widehat{J}(u) := J(y(u), u) \quad \text{s. t.} \quad u \in U_{ad},$$

Trust region method:

$u_{k+1} = u_k + s_k$, where s_k is an approximate solution of the

Trust region problem at u_k:

$$\min_{s \in U} \ \widehat{q}_k(s) := \widehat{J}(u_k) + (\widehat{g}_k, s)_U + \frac{1}{2}\langle s, \widehat{H}_k s\rangle_{U,U^*}$$
$$\text{s. t.} \quad u_k + s \in U_{ad}, \quad \|s\|_U \le \delta_k$$

- $\widehat{g}_k$ reduced gradient: Riesz representation of $\widehat{J}'(u_k) = L_u(y_k, u_k, \lambda_k)$
- y_k solves state eq. $C(y_k, u_k) = 0$, λ_k solves adjoint eq. $L_y(y_k, u_k, \lambda_k) = 0$
- $\widehat{H}_k$ approximation of reduced Hessian $\widehat{J}''(u_k)$
- $\delta_k > 0$ trust region radius (adjusted by the trust region method)

Basic Trust Region Method 2

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Choose $0 < \eta_1 < \eta_2 < 1$ and initial $u_0 \in U_{ad}$. Set $k := 0$.

1. Compute state $y_k = y(u_k)$, i.e. $C(y_k, u_k) = 0$.
2. Compute adjoint state λ_k, i.e. $L_y(y_k, u_k, \lambda_k) = 0$.
3. Compute reduced gradient $\widehat{g}_k$ as Riesz representation of $L_u(y_k, u_k, \lambda_k)$.
3. If $\|u_k - P_{U_{ad}}(u_k - \widehat{g}_k)\|_U \le \varepsilon_{tol}$: STOP
4. Compute s_k as inexact solution of the trust region problem

$$\boxed{\min \quad \widehat{q}_k(s) \quad \text{subject to} \quad \|s\|_U \le \delta_k, u_k + s \in U_{ad}.}$$

5. Compute new state $y_{k+1} = y(u_k + s_k)$.
6. **Accept or Reject Step:** If

$$\frac{J(y_k, u_k) - J(y_{k+1}, u_{k+1})}{\widehat{q}_k(0) - \widehat{q}_k(s_k)} \begin{cases} \ge \eta_1 & (u_{k+1}, y_{k+1}) := (u_k + s_k, y_{k+1}),\ \delta_{k+1} := \delta_k, \\ \ge \eta_2 & (u_{k+1}, y_{k+1}) := (u_k + s_k, y_{k+1}),\ \delta_{k+1} > \delta_k, \\ < \eta_1 & (u_{k+1}, y_{k+1}) := (u_k, y_k),\ \delta_{k+1} := \delta_k/2. \end{cases}$$

$k \leftarrow k + 1$. Goto 1.

Multilevel Trust Region Algorithm: Discretization

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We assume for simplicity a conformal discretization:

$$Y_h \subset Y, \quad U_h \subset U, \quad \Lambda_h \subset \Lambda,$$

Let in iteration k a current grid and a control $u_k \in U_{h_k}$ be given.

Discretized state equation:

Compute $y_k = y_k^{h_k} \in Y_{h_k}$ by applying a convergent solver of $C(y, u_k) = 0$

$$C^{h_k} : Y_{h_k} \times U_{h_k} \to \Lambda_{h_k}^*, \qquad C^{h_k}(y_k, u_k) = 0.$$

Discretized adjoint equation:

Compute $\lambda_k = \lambda_k^{h_k} \in \Lambda_{h_k}$ by applying a convergent solver of $L_y(y_k, u_k, \lambda) = 0$.

Discrete reduced gradient:

$$\widehat{g}_k = \text{Riesz representation of } L_u(y_k, u_k, \lambda_k) \text{ in } U_h.$$

Criticality Measure

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$U_{ad} \subset U$ closed, convex, $P_{U_{ad}}$ projection onto U_{ad}.

Criticality measure:

$$\|Pg_k\|_U := \|u_k - P_{U_{ad}}(u_k - \widehat{g}_k)\|_U$$

Discrete criticality measure:

$$\|P^h g_k\|_{U_h} := \|u_k - P^h_{U^h_{ad}}(u_k - \widehat{g}_k)\|_{U_h}$$

$P^h_{U^h_{ad}}$ projection onto U^h_{ad}.

Example: $U_{ad} = \{u \in U : a \le u \le b\}, \quad a, b \in L^\infty,\ a \le b.$

$$P_{U_{ad}}(u_k - \widehat{g}_k) = \max(a, \min(u_k - \widehat{g}_k, b))$$

Adaptive Multilevel Trust Region Algorithm

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Choose initial discretization (P^{h_0}), $u_0 \in U_{ad}^{h_0}$. Set $k := 0$.

1. Compute discrete state y_k (sufficiently) exactly (if not already done).
2. Compute a discrete adjoint state λ_k, inexact reduced gradient $\widehat{g}_k$.

R1. Estimate $\|C(y_k, u_k)\|_{\Lambda^*}$ and compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grid for Y_{h_k}, Λ_{h_k} adaptively. Goto 1.)

R2. Estimate $\|L_y(y_k, u_k, \lambda_k)\|_{Y^*}$, $\|Pg_k - P^{h_k} g_k\|_U$, compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grids adaptively. Goto 1.)

3. If $\|P^{h_k} g_k\|_{U_{h_k}} \leq \varepsilon_{tol}$: STOP
4. Compute s_k as inexact solution of

$$\min \quad \widehat{q}_k^{h_k}(s) \quad \text{subject to} \quad \|s\|_{U_{h_k}} \leq \delta_k, u_k + s \in U_{ad}^{h_k}.$$

5. Compute discrete state $y_{k+1} = y^{h_k}(u_k + s_k)$ (sufficiently) exactly.
6. Accept or reject step by reduction ratio, choose δ_{k+1}. $k \leftarrow k + 1$. Goto 1.
If rejected, check inexact reduced gradient $\widehat{g}_k$, possibly refine and go to 1.

Outline

- Problem setting and basic concept
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- Extension to reduced order models with error estimation
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Adaptive Multilevel Trust Region Algorithm

Choose initial discretization (P^{h_0}), $u_0 \in U_{ad}^{h_0}$. Set $k := 0$.

1. Compute discrete state y_k (sufficiently) exactly (if not already done).
2. Compute a discrete adjoint state λ_k, inexact reduced gradient $\widehat{g}_k$.

R1. Estimate $\|C(y_k, u_k)\|_{\Lambda^*}$ and compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grid for Y_{h_k}, Λ_{h_k} adaptively. Goto 1.)

R2. Estimate $\|L_y(y_k, u_k, \lambda_k)\|_{Y^*}$, $\|P g_k - P^{h_k} g_k\|_U$, compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grids adaptively. Goto 1.)

3. If $\|P^{h_k} g_k\|_{U_{h_k}} \le \varepsilon_{tol}$: STOP
4. Compute s_k as inexact solution of

$$\boxed{\min \quad \widehat{q}_k^{h_k}(s) \quad \text{subject to} \quad \|s\|_{U_{h_k}} \le \delta_k, u_k + s \in U_{ad}^{h_k}.}$$

5. Compute discrete state $y_{k+1} = y^{h_k}(u_k + s_k)$ (sufficiently) exactly.
6. Accept or reject step by reduction ratio, choose δ_{k+1}. $k \leftarrow k + 1$. Goto 1.
If rejected, check inexact reduced gradient $\widehat{g}_k$, possibly refine and go to 1.

Adaptive Multilevel Trust Region Algorithm

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Choose initial discretization (P^{h_0}), $u_0 \in U_{ad}^{h_0}$. Set $k := 0$.

1. Compute discrete state y_k (sufficiently) exactly (if not already done).
2. Compute a discrete adjoint state λ_k, inexact reduced gradient $\widehat{g}_k$.

R1. Estimate $\|C(y_k, u_k)\|_{\Lambda^*}$ and compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grid for Y_{h_k}, Λ_{h_k} adaptively. Goto 1.)

R2. Estimate $\|L_y(y_k, u_k, \lambda_k)\|_{Y^*}$, $\|P g_k - P^{h_k} g_k\|_U$, compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grids adaptively. Goto 1.)

3. If $\|P^{h_k} g_k\|_{U_{h_k}} \leq \varepsilon_{tol}$: STOP
4. Compute s_k as inexact solution of

$$\min \quad \widehat{q}_k^{h_k}(s) \quad \text{subject to} \quad \|s\|_{U_{h_k}} \leq \delta_k, u_k + s \in U_{ad}^{h_k}.$$

5. Compute discrete state $y_{k+1} = y^{h_k}(u_k + s_k)$ (sufficiently) exactly.
6. Accept or reject step by reduction ratio, choose δ_{k+1}. $k \leftarrow k + 1$. Goto 1.
   If rejected, check inexact reduced gradient $\widehat{g}_k$, possibly refine and go to 1.

Refinement Criteria

Step R1,R2: Estimate residuals in optimality conditions

Implement with fixed (unknown) constants $K_y, K_\lambda, K_u > 0$ the following criteria:

Check if

$$\begin{aligned}
\|C(y_k, u_k)\|_{\Lambda^*} &\leq K_y \|P^{h_k} g_k\|_{U_{h_k}} \\
\|L_y(y_k, u_k, \lambda_k)\|_{Y^*} &\leq K_\lambda \|P^{h_k} g_k\|_{U_{h_k}} \\
\|P g_k - P^{h_k} g_k\|_U &\leq K_u \|P^{h_k} g_k\|_{U_{h_k}}
\end{aligned}$$

Otherwise refine the grid for Y_{h_k}, Λ_{h_k}, U_{h_k} and goto Step 1.

Refinement Criteria

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Implement with fixed (unknown) constants $K_y, K_\lambda, K_u > 0$ the following criteria:

Check if

$$\begin{aligned} \|C(y_k, u_k)\|_{\Lambda^*} &\le K_y \|P^{h_k} g_k\|_{U_{h_k}} \\ \|L_y(y_k, u_k, \lambda_k)\|_{Y^*} &\le K_\lambda \|P^{h_k} g_k\|_{U_{h_k}} \\ \|P g_k - P^{h_k} g_k\|_U &\le K_u \|P^{h_k} g_k\|_{U_{h_k}} \end{aligned}$$

Otherwise refine the grid for Y_{h_k}, Λ_{h_k}, U_{h_k} and goto Step 1.

Assume that we have reliable error estimators $\eta_{y,h}$, $\eta_{\lambda,h}$, $\eta_{Pg,h}$ with

$$\begin{aligned} \|C(y_k, u_k)\|_{\Lambda^*} &\le C_1 \eta_{y,h_k} \\ \|L_y(y_k, u_k, \lambda_k)\|_{Y^*} &\le C_2 \eta_{\lambda,h_k} \\ \|P g_k - P^{h_k} g_k\|_U &\le C_3 \eta_{Pg,h_k} \end{aligned}$$

Refinement Criteria

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Step R1,R2: Estimate residuals in optimality conditions

Implement with fixed constants $\tilde{K}_y, \tilde{K}_\lambda, \tilde{K}_u > 0$ the following criteria:

Check if

$$\begin{aligned} \eta_{y,h_k} &\leq \tilde{K}_y \| P^{h_k} g_k \|_{U_{h_k}} \\ \eta_{\lambda,h_k} &\leq \tilde{K}_\lambda \| P^{h_k} g_k \|_{U_{h_k}} \\ \eta_{Pg,h_k} &\leq \tilde{K}_u \| P^{h_k} g_k \|_{U_{h_k}} \end{aligned}$$

Otherwise refine the grid for Y_{h_k}, Λ_{h_k}, U_{h_k} and goto Step 1.

Assume that we have reliable error estimators $\eta_{y,h}$, $\eta_{\lambda,h}$, $\eta_{Pg,h}$ with

$$\begin{aligned} \| C(y_k, u_k) \|_{\Lambda^*} &\leq C_1 \eta_{y,h_k} \\ \| L_y(y_k, u_k, \lambda_k) \|_{Y^*} &\leq C_2 \eta_{\lambda,h_k} \\ \| P g_k - P^{h_k} g_k \|_U &\leq C_3 \eta_{Pg,h_k} \end{aligned}$$

Adaptive Multilevel Trust Region Algorithm

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Choose initial discretization (P^{h_0}), $u_0 \in U_{ad}^{h_0}$. Set $k := 0$.

1. Compute discrete state y_k (sufficiently) exactly (if not already done).
2. Compute a discrete adjoint state λ_k, inexact reduced gradient $\widehat{g}_k$.

R1. Estimate $\|C(y_k, u_k)\|_{\Lambda^*}$ and compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grid for Y_{h_k}, Λ_{h_k} adaptively. Goto 1.)

R2. Estimate $\|L_y(y_k, u_k, \lambda_k)\|_{Y^*}$, $\|Pg_k - P^{h_k} g_k\|_U$, compare with $\|P^{h_k} g_k\|_{U_{h_k}}$.
(If ratio too large, refine grids adaptively. Goto 1.)

3. If $\|P^{h_k} g_k\|_{U_{h_k}} \leq \varepsilon_{tol}$: STOP
4. Compute s_k as inexact solution of

$$\min \quad \widehat{q}_k^{h_k}(s) \quad \text{subject to} \quad \|s\|_{U_{h_k}} \leq \delta_k, u_k + s \in U_{ad}^{h_k}.$$

5. Compute discrete state $y_{k+1} = y^{h_k}(u_k + s_k)$ (sufficiently) exactly.
6. Accept or reject step by reduction ratio, choose δ_{k+1}. $k \leftarrow k + 1$. Goto 1.
If rejected, check inexact reduced gradient $\widehat{g}_k$, possibly refine and go to 1.

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If rejected, check inexact reduced gradient $\widehat{g}_k$, possibly refine and go to 1.

Trust Region Step

Step 4: Compute s_k as inexact solution of

$$\begin{aligned} &\min \quad \widehat{q}_k^{h_k}(s) = J(y_k, u_k) + (\widehat{g}_k^{h_k}, s)_{U_{h_k}} + \frac{1}{2}\left\langle s, \widehat{H}_k^{h_k} s \right\rangle_{U_{h_k}, U_{h_k}^*} \\ &\text{subject to} \quad \|s\|_U \leq \delta_k, u_k + s \in U_{ad}^{h_k}. \end{aligned}$$

that satisfies the **Generalized Cauchy decrease condition**

$$\widehat{q}_k^{h_k}(0) - \widehat{q}_k^{h_k}(s_k) \geq \kappa_q \|P^{h_k} g_k\|_{U_{h_k}} \min\{\|P^{h_k} g_k\|_{U_{h_k}}, \delta_k\}.$$

with $\kappa_q \in (0, 1)$

Possibilities: e.g.

- Projected negative gradient direction with Armijo linesearch (works always if Hessians are bounded, $\|H_k^{h_k}\| \leq R$, $R > 0$)
- Projected pcg-Newton step with Armijo linesearch

Adaptive Multilevel Trust Region Algorithm

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Adaptive Multilevel Trust Region Algorithm

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Refinement Criterion for Inexact Reduced Gradient

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In our "first optimize then discretize" approach we allow:

Independent adjoint solver for adjoint PDE

$\rightsquigarrow$ inexact reduced gradient $\widehat{g}_k$

Implement with arbitrary constant $\xi > 0$ the following criterion:

In Step 6: If step is not acceptable then check

$$|(\widehat{g}_k, s_k)_{U_{h_k}} - \langle \nabla \widehat{J}(u_k), s_k \rangle| \leq \xi \min\{\|P^{h_k} g_k\|_{U_{h_k}}, \delta_k\} \|s_k\|_{U_{h_k}}.$$

Otherwise refine the grids and go to step 1.

Criterion for Mesh Adaptation

Use a refinement strategy such that

$$\sum_{k=0}^{\infty}\left(J(y_{k+1}^{h_{k+1}}, u_{k+1}^{h_k}) - J(y_{k+1}^{h_k}, u_{k+1}^{h_k})\right) < \infty.$$

Meaning:

- Refine such that continuous problem is approached sufficiently fast
- Results of Nochetto, Siebert et al. indicate that standard refinement techniques satisfy the condition

Convergence Result

Theorem: (Ziems, S.U. SIOPT 2011, Ziems SIOPT 2013)

If standard assumptions hold uniformly on all generated grids then

- for $\varepsilon_{tol} > 0$ the adaptive multilevel trust region method with the given refinement criteria terminates finitely and
- for $\varepsilon_{tol} = 0$ the algorithm terminates finitely with a stationary point or produces a sequence with $u_k \in U_{ad}$, $k \in \mathbb{N}$, and

$$\liminf_{k\to\infty} \|C(y_k, u_k)\|_{\Lambda^*} + \|L_y(y_k, u_k, \lambda_k)\|_{Y^*} + \|P\widehat{g}_k\|_U = 0.$$

Local Refinement Strategy

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Based on Elementwise Contributions to Error Estimators:

$$\eta_{C,h} = \left(\sum_{\text{Elements } T \text{ in triangulation}} \eta_{C,h,T}^2 \right)^{1/2}$$

$$\eta_{L_y,h} = \left(\sum_{\text{Elements } T \text{ in triangulation}} \eta_{L_y,h,T}^2 \right)^{1/2}$$

Typical Example for Refinement Strategy:

- **State:** Refine the $p\%$ elements with largest local errors $\eta_{C,h,T}$.
- **Adjoint:** Refine the $p\%$ elements with largest local errors $\eta_{L_y,h,T}$.

Suitable error estimators: e.g., Bank, Bartels, Becker, Carstensen, Funken, Hoppe, Rannacher, Siebert, Süli, Zienkiewicz, Zhu, ...

Outline

- Problem setting and basic concept
- Adaptive multilevel methods for time-dependent PDE-constrained optimization with control constraints
- Implementation of the error control criteria by error estimators
- Extension to reduced order models with error estimation
- Numerical results

Basic Idea for Including Reduced Order Models

- Approximate current adaptive FE-discretization by ROM.
- Compute optimization steps with the ROM by using the same adaptive optimization method as before (now: FE-model instead of PDE-model, ROM instead of FE-model).
- Estimate error between state/adjoint FE-model and state/adjoint ROM (e.g., Grepl, Patera 2005; Haasdonk, Ohlberger 2006; Tröltzsch, Volkwein 2009; Urban, Patera 2012).
- Instead of mesh refinement improve ROM.
- If ROM requires improvement, check if FE-model itself needs refinement.
- If necessary, refine FE-model adaptively as before and update the ROM.

For simplicity:

On the ROM level we use exact discrete adjoints, i.e. exact reduced gradients.

Example: Reduced Order Models by Proper Orthogonal Decomposition

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- Let $C(y, u) = 0$ be given by

$$\langle y_t(t), v \rangle_{V^*,V} + a(y(t), v) = \langle Bu(t), v \rangle_{V^*,V} \quad \forall\, v \in V, t \in (0, T), \quad y(0) = y_0.$$

- **FE-Discretization (impl. Euler):** Find $y^{fe}(t_i) \in V_h$ with $y^{fe}(t_0) = y_{0,h}$,

$$\left\langle \frac{y^{fe}(t_i) - y^{fe}(t_{i-1})}{\Delta t_i}, v_h \right\rangle_{V_h^*,V_h} + a(y^{fe}(t_i), v_h) = \langle Bu(t_i), v_h \rangle_{V_h^*,V_h} \quad \forall\, v_h \in V_h.$$

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- **Construction of POD-Basis:**
  For the span of snapshots $S = \text{span}\{y^{fe}(t_1), \dots, y^{fe}(t_N)\}$ generate an ONB $\{\varphi_1, \dots, \varphi_m\}$ (POD-Basis) w.r.t. some $(\cdot,\cdot)_H$, such that $\text{span}\{\varphi_1, \dots, \varphi_l\}$, $l \le m$, is best approximation with dimension l of the snapshots.
- Choose l and set $V_h^r := \text{span}\{\varphi_1, \dots, \varphi_l\}$
- **POD-ROM (impl. Euler):** Find $y^r(t_i) \in V_h^r$ with $y^r(t_0) = y_{0,h}^r$,

$$\left\langle \frac{y^r(t_i) - y^r(t_{i-1})}{\Delta t_i}, \varphi_j \right\rangle_{V_h^*,V_h} + a(y^r(t_i), \varphi_j) = \langle Bu(t_i), \varphi_j\rangle_{V_h^*,V_h}, \quad j = 1, \dots, l.$$

Adaptive Multilevel Trust Region Algorithm with Reduced Order Models

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Choose (P^{h_0}), $u_0 \in U_{ad}^{h_0}$. Set $k := 0$. Setup initial state /adjoint ROMs.

1. Compute discrete FE state y_k^{fe} (sufficiently) exactly (if not already done).
2. Compute a discrete FE adjoint state λ_k^{fe}, inexact reduced gradient $\widehat{g}_k^{fe}$.

R1. Estimate $\|C(y_k^{fe}, u_k)\|_{\Lambda^*}$ and compare with $\|P^{h_k} g_k^{fe}\|_{U_{h_k}}$.
(If ratio too large, refine grid for Y_{h_k}, Λ_{h_k} adaptively. Goto 1.)

R2. Estimate $\|L_y(y_k^{fe}, u_k, \lambda_k^{fe})\|_{Y^*}$, $\|P g_k^{fe} - P^{h_k} g_k^{fe}\|_U$, compare with $\|P^{h_k} g_k^{fe}\|_{U_{h_k}}$.
(If ratio too large, refine grids adaptively. Goto 1.)

3. If $\|P^{h_k} g_k^{fe}\|_{U_{h_k}} \leq \varepsilon_{tol}$: STOP

Adaptive Multilevel Trust Region Algorithm with Reduced Order Models

TECHNISCHE UNIVERSITÄT DARMSTADT

Choose (P^{h_0}), $u_0 \in U_{ad}^{h_0}$. Set $k := 0$. Setup initial state /adjoint ROMs.

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(If ratio too large, refine grid for Y_{h_k}, Λ_{h_k} adaptively. Goto 1.)

R2. Estimate $\|L_y(y_k^{fe}, u_k, \lambda_k^{fe})\|_{Y^*}$, $\|P g_k^{fe} - P^{h_k} g_k^{fe}\|_U$, compare with $\|P^{h_k} g_k^{fe}\|_{U_{h_k}}$.
(If ratio too large, refine grids adaptively. Goto 1.)

3. If $\|P^{h_k} g_k^{fe}\|_{U_{h_k}} \leq \varepsilon_{tol}$: STOP

ROM.1. Compute ROM state y_k^r exactly (if not already done).

ROM.2. Compute ROM adjoint state λ_k^r, reduced ROM gradient $\widehat{g}_k^r$.

ROM.R. If estimator$(\|C^{h_k}(y_k^r, u_k)\|_{\Lambda_{h_k}^*} \|L_y^{h_k}(y_k^r, u_k, \lambda_k^r)\|_{Y_{h_k}^*}) >$
$\min(K_r \|P^{h_k,r} g_k^r\|_{U_{h_k}}^2, \kappa_C \mathrm{Tol}^2)$ or if $\|P^{h_k,r} g_k^r\|_{U_{h_k}} \leq \varepsilon_{tol}^r$:

- Check and possibly improve FE-model by calling steps 1–3.
- Improve state/adjoint ROM. Set $\mathrm{Tol} := \mathrm{Tol}/2$. Goto ROM.1.

Adaptive Multilevel Trust Region Algorithm with Reduced Order Models

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1.–3. ...

ROM.1. Compute ROM state y_k^r exactly (if not already done).

ROM.2. Compute ROM adjoint state λ_k^r, reduced ROM gradient $\widehat{g}_k^r$.

ROM.R. If estimator$(\|C^{h_k}(y_k^r, u_k)\|_{\Lambda_{h_k}^*} \|L_y^{h_k}(y_k^r, u_k, \lambda_k^r)\|_{Y_{h_k}^*}) >$ $\min(K_r \|P^{h_k,r} g_k^r\|_{U_{h_k}}^2, \kappa_C \mathrm{Tol}^2)$ or if $\|P^{h_k,r} g_k^r\|_{U_{h_k}} \leq \varepsilon_{tol}^r$:

- Check and possibly improve FE-model by calling steps 1–3.
- Improve state/adjoint ROM. Set Tol := Tol/2. Goto ROM.1.

ROM.3. Compute s_k as inexact solution of the ROM-based problem

$$\min \quad \widehat{q}_k^{h_k,r}(s) \quad \text{subject to} \quad \|s\|_{U_{h_k}} \leq \delta_k, u_k + s \in U_{ad}^{h_k}.$$

ROM.4. Compute ROM state $y_{k+1}^r = y^{h_k,r}(u_k + s_k)$ exactly.

ROM.5. Accept/reject step, choose δ_{k+1}. $k \leftarrow k + 1$. Goto ROM.1.

Observations and Features

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- One can show that

$$|J(y^{h_k}(u),u) - J(y^{h_k,r}(u),u)| \le c\|C^{h_k}(y_k^r,u_k)\|_{\Lambda_{h_k}^*}\|L_y^{h_k}(y_k^r,u_k,\lambda_k^r)\|_{Y_{h_k}^*} + \text{H.O.T.}$$

$$J(y^{h_k,r}(u_k),u_k) - J(y^{h_k,r}(u_{opt}),u_{opt}) \ge c\|P^{h_k,r}g_k^r\|_{U_{h_k}}^2$$

  This motivates the criterion

$$\text{estimator}(\|C^{h_k}(y_k^r,u_k)\|_{\Lambda_{h_k}^*}\|L_y^{h_k}(y_k^r,u_k,\lambda_k^r)\|_{Y_{h_k}^*}) > \min(K_r\|P^{h_k,r}g_k^r\|_{U_{h_k}}^2, \kappa_C \text{Tol}^2)$$

- Convergence properties remain the same as for FE-based method.
- For nonlinear problems, application of Discrete Empirical Interpolation is helpful to obtain efficient POD-based ROMs (Barrault, Maday, Nguyen, Patera 2004, Chaturantabut, Sorensen 2010).
- Steps are computed based on the ROM, hence second order methods ($\widehat{H}_k = (\widehat{J}^r)''(u_k)$) are not expensive.

Related work: Pironneau, Polak 2000; Arian, Fahl, Sachs 2000, Volkwein 2011.

A Posterior Error Estimators for ROMs

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Error Estimators:

- Residuals $\|C^{h^k}(y_k^r, u_k)\|_{\Lambda^*_{h_k}}$, $\|L_y^{h^k}(y_k^r, u_k, \lambda_k^r)\|_{Y^*_{h_k}}$ directly computable.
- Error is often devided in space- and time-errors (Debrabant, Lang 09).
- To avoid computations on the FE-grid, one can prepare the spatial residual computation "offline" to speed up later frequent evaluations (e.g., Grepl, Patera; Canuto, Tonn, Urban; Haasdonk, Ohlberger; Urban, Patera; Quarteroni, Rozza, Iapichino et al.).

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Model Improvement Strategies:

- Include snapshots of the state/adjoint for the current control.
- Maximize the ROM error estimator w.r.t. the control and include corresponding state snapshots Patera; deVore; Canuto, Tonn, Urban et al.; Quarteroni, Rozza, Iapichino et al.
- Further approaches e.g. by Arian, Fahl, Sachs 2006; Afanasiev, Hinze 2001; Volkwein 2011; Ghiglieri, S.U. 2012.

Extension to State Constraints

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PDE-constrained Optimization Problem (PS):

$$\min_{y \in Y, u \in U} \; J(y,u) \quad \text{subject to} \quad C(y,u) = 0, \quad u \in U_{ad}, \quad y \in Y_{ad}.$$

$Y \subset \mathcal{C}^0(Q)$	State space,	$U_{ad} \subset U$	Convex, closed set,
U	Control space (Hilbert space),	$J : Y \times U \to \mathbb{R}$	Objective function,
		$C : Y \times U_{ad} \to \Lambda^*$	State equation.

$Y_{ad} = \{y \in \mathcal{C}^0(Q) \,:\, y_a \le y \le y_b\}$,
$y_a, y_b \in \mathcal{C}^0(Q)$, $y_a < y_b$.

Moreau-Yosida Regularization

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Regularized Optimization Problem $(\mathrm{PS})_\gamma$:

$$\min_{y\in Y, u\in U} \quad J_\gamma(y,u) := J(y,u) + \gamma\left(\|(y_a - y)_+\|^3_{L^3(Q)} + \|(y - y_b)_+\|^3_{L^3(Q)}\right)$$

$$\text{subject to} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

γ Regularization parameter

$(y_a - y)_+ = \max(0, y_a - y)$

Bergounioux, Hintermüller, Hinze, Kunisch, Meyer, Neitzel, Rösch, Tröltzsch, M. Ulbrich, Yousept,...

Extension of the Adapative Multilevel Method to State Contraints

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$$\min_{y\in Y, u\in U} \quad J^\gamma(y,u) := J(y,u) + \gamma\left(\|(y_a - y)_+\|^3_{L^3(Q)} + \|(y-y_b)_+\|^3_{L^3(Q)}\right)$$
$$\text{subject to} \quad C(y,u) = 0, \quad u \in U_{ad}.$$

Notation: Let $a : \mathbb{R}_+ \to \mathbb{R}+$ be strictly monotone decreasing, $\lim_{\gamma\to\infty} a(\gamma) = 0$

- Apply the multilevel algorithm to $(\mathrm{PS})_{\gamma_k}$ while adjusting γ_k.
- Refine the grid if one of the following conditions is violated

$$\begin{aligned}
\eta_{y,h_k} &\le \tilde{K}_y \max(\|P^{h_k} g_k^{\gamma_k}\|_{U_{h_k}}, c_y a(\gamma_k)) \\
\eta_{\lambda,h_k} &\le \tilde{K}_\lambda \max(\|P^{h_k} g_k^{\gamma_k}\|_{U_{h_k}}, c_\lambda a(\gamma_k)) \\
\eta_{Pg,h_k} &\le K_u \max(\|P^{h_k} g_k^{\gamma_k}\|_{U_{h_k}}, c_u a(\gamma_k))
\end{aligned}$$

- Increase γ_k if $a(\gamma_k) > K_a \|P^{h_k} g_k^{\gamma_k}\|_{U_{h_k}}$

Convergence analysis: Bott, S.U., Ziems 2012

Outline

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- Problem setting and basic concept
- Adaptive multilevel methods for time-dependent PDE-constrained optimization with control constraints
- Implementation of the error control criteria by error estimators
- Extension to reduced order models with error estimation
- Numerical results

Numerical Results for Parabolic Problem with Control Constraints

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Test Problem: Boundary Control of semilinear parabolic PDE

$$\min J(y,u) := \frac{1}{2}\|y(T)-y_d\|^2_{L^2(\Omega)} + \frac{1}{2}\|y-y_Q\|^2_{L^2(Q)} + \frac{\alpha}{2}\|u\|^2_{L^2((0,T)\times\partial\Omega)}$$

$$\text{subject to} \quad \begin{aligned} & y_t - \Delta y + y^3 = 0 \quad \text{in } Q := (0,T)\times\Omega, \\ & \partial_n y = u - y^4 \quad \text{on } (0,T)\times\partial\Omega, \\ & y(0) = y_0 \quad \text{in } \Omega \\ & a \le u \le b \end{aligned}$$

$\Omega = [0,1]\times[0,1]$ unit square,
$T = 1$, $\alpha = 0.01$,
$y_0 \equiv 1$, $y_d \equiv 0.2$, $y_Q(t) \equiv 1 - 0.8t$,
$a \equiv 0$, $b \equiv 0.4$

Iteration History

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Algorithm with ROM (POD-DEIM):

It.	Ref.	$\eta_{y,h}[t,s]$	$\eta_{\lambda,h}[t,s]$	$\|\widetilde{P}^h g_k\|_U$	(t,x)-grid	POD, DEIM
0		1.8e-4 , 4.6e-3	8.5e-3 , 5.7e-3	2.6e-1	36 × 289	14, 16
1		2.7e-4 , 9.4e-3	3.0e-2 , 2.8e-3	4.9e-2	36 × 289	14, 16
	λ t	2.9e-4 ,	1.0e-4 ,	4.9e-2	67 × 289	14, 17
5		9.7e-4 , 1.1e-2	7.2e-6 , 1.5e-4	1.0e-3	67 × 289	14, 17
	y s,t	2.1e-4 , 1.7e-3	1.1e-6 , 2.3e-5	1.1e-3	157 × 1089	24, 30
11	y s,t	3.3e-5 , 1.5e-3	9.6e-7 , 4.5e-5	1.5e-4	157 × 1089	24, 30
14		2.1e-5 , 1.6e-3	9.4e-7 , 4.7e-5	7.0e-5	157 × 1089	24, 30
	y s,t	1.3e-5 , 7.7e-4	6.2e-6 , 8.6e-6	4.3e-5	217 × 4225	
	y s,t	3.1e-6 , 1.9e-4	4.4e-6 , 2.0e-6	4.8e-5	438 × 16641	24, 33
19		1.2e-6 , 2.6e-4	8.4e-8 , 3.1e-5	2.1e-5	438 × 16641	24, 33
	ROM	1.3e-6 , 2.2e-4	8.4e-8 , 3.1e-5	1.3e-4	438 × 16641	49, 33
23		8.0e-7 , 2.2e-4	8.4e-8 , 3.1e-5	2.0e-5	438 × 16641	49, 33
	ROM	8.3e-7 , 1.7e-4	8.4e-8 , 3.1e-5	2.0e-5	438 × 16641	74, 33
24		8.4e-7 , 1.7e-4	8.4e-8 , 3.1e-5	7.9e-6	438 × 16641	74, 33
	ROM	8.9e-7 , 1.9e-4	1.0e-6 , 2.0e-6	7.9e-6	438 × 16641	122, 33
		9.6e-7 , 1.9e-4	1.8e-6 , 2.0e-6	7.9e-6	438 × 16641	

Algorithm without ROM:

similar grids: 36 , 67 , 156 , 216 , 441 points in time, same spatial grids.

23	STOP	9.5e-7 , 1.9e-4	1.7e-7 , 2.0e-6	8.2e-6	441 × 16641

Adaptive Multilevel Method with ROM: Efficiency

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Adaptive POD-DEIM, only boundary nonlinearity y^4:

(time optimization)/(time state simulation on last grid) $= 3.7$

Adaptive POD-DEIM, boundary nonlinearity y^4 and distributed nonlinearity y^3:

(time optimization)/(time state simulation on last grid) $= 3.85$

We observe similar performance for flow control problems.

Application: Optimal Glass Cooling

- Cooperation with J. Lang, D. Clever and J.C. Ziems within SPP 1253
- Quality control of complex glass production processes
- Avoid cracks and other defects
- High temperature $\rightarrow$ radiation has to be taken into account
- Discretization of the state and adjoint equation with the space-time adaptive solver KARDOS (Lang, Clever)

Modelling of Radiative Heat Transfer

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Temperature $T(x,t)$ and Intensity $I(x,t,\nu,s)$:

$$\begin{aligned} \rho_m\, c_m\, \partial_t T - \nabla \cdot (k_c \nabla T) &= -\int_{\nu_0}^{\infty} \int_{S^2} \kappa\,(\,B_m(T,\nu) - I\,)\, ds\, d\nu \\ \forall \nu > \nu_0 : \quad s \cdot \nabla I + (\sigma + \kappa) I &= \frac{\sigma}{4\pi} \int_{S^2} I\, ds + \kappa\, B_m(T,\nu) \end{aligned}$$

$$B_m(T,\nu) = \frac{n_m^2}{c_0^2} \frac{2\, h_P\, \nu^3}{e^{h_p \nu/(k_B T)} - 1} \quad \text{(Planck function)}$$

$x \in \Omega$ space, $t \in [0, t_e]$ time, $\nu \in (0, \infty)$ frequency, $s \in S^2$ direction
Control: ambient temperature $u(t)$.

Coupling with KARDOS

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Gray Scale Glass cooling problem (Pinnau, Klar, Thömmes, et al.)

$$\min \frac{1}{2}\int_0^{t_e} \|T - T_d\|^2_{L^2(\Omega)} dt + \frac{\delta_e}{2}\|(T - T_d)(t_e)\|^2_{L^2(\Omega)} + \frac{\delta_u}{2}\int_0^{t_e} \|u - u_d\|^2_{L^2(\partial\Omega)} dt$$

s.t.

$$\begin{aligned}
\partial_t T - k\Delta T - \frac{1}{3\kappa}\Delta\phi &= 0 && \text{in } \Omega \times (0, t_e] \\
-\frac{\epsilon^2}{3\kappa}\Delta\phi &= -\kappa\phi + 4\pi\kappa a T^4 && \text{in } \Omega \times (0, t_e] \\
kn \cdot \nabla T + \frac{1}{3\kappa} n \cdot \nabla\phi &= \frac{h}{\epsilon}(u - T) + \frac{1}{2\epsilon}4\pi a u^4 - \frac{1}{2\epsilon}\phi && \text{in } \partial\Omega \times (0, t_e] \\
\frac{\epsilon^2}{3\kappa} n \cdot \nabla\phi &= \frac{\epsilon}{2}(4\pi a u^4 - \phi) && \text{in } \partial\Omega \times (0, t_e] \\
T(0, x) &= T_0(x) && \text{in } \Omega
\end{aligned}$$

3D Optimal Control of Glass Cooling

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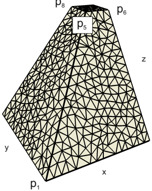
Iteration history of the Second Order Multilevel Optimization Method



iteration	objective value	criticality measure	computing time
0	1.4602e+03	4.0245e+01	0.01%
1	5.4880e+02	2.8733e+00	0.04%
1	5.5664e+02	2.9758e+00	0.04%
2	5.4908e+02	3.4451e-01	0.35%
2	5.4507e+02	9.5386e-01	0.07%
3	5.4478e+02	3.0787e-01	1.05%
3	5.5319e+02	5.4405e-01	0.50%
4	5.5302e+02	1.0118e-01	9.96%
4	5.6995e+02	8.5377e-01	2.84%
5	5.6997e+02	6.8337e-02	85.10%

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3D Optimal Control of Glass Cooling

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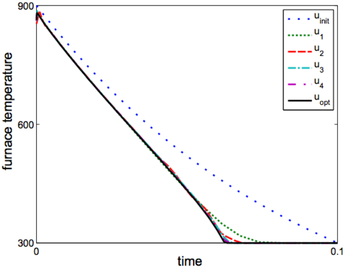
Control iterates u_k, $k = 0, \dots, 5$



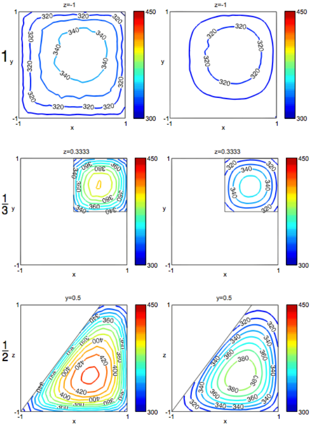
Initial space-time-grid: 25.000 DOF
Final space-time-grid: 1.755.000 DOF

Initial glass temperature Optimal glass temperature

$z = 1$

$z = \frac{1}{3}$

$y = \frac{1}{2}$



Thermistor Problem with State Constraints

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Cf. Hömberg, Meyer, Rehberg, Ring; Meyer, Meinlschmidt

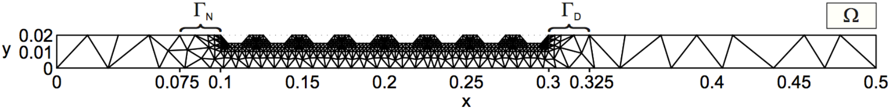
$$\min \frac{1}{2}\int_0^{t_e} \|T - T_d\|^2_{L^2(\Omega)}\,\mathrm{d}t + \frac{\delta_e}{2}\|(T - T_d)(t_e)\|^2_{L^2(\Omega)} + \frac{\delta_u}{2}\int_0^{t_e}(u - u_d)^2\mathrm{d}t$$

$$\begin{aligned}
\text{s.t.}\ \ C\rho\partial_t T - \nabla\cdot(\kappa\nabla T) &= (\sigma(T)\nabla\phi)\cdot\nabla\phi && \text{in } \Omega\times(0,t_e]\\
-\nabla\cdot(\sigma(T)\nabla\phi) &= 0 && \text{in } \Omega\times(0,t_e]\\
n\cdot(\kappa\nabla T) &= \alpha(T_l - T) && \text{in } \partial\Omega\times(0,t_e]\\
n\cdot(\sigma(T)\nabla\phi) &= C_u u && \text{in } \partial\Omega_N\times(0,t_e]\\
n\cdot(\sigma(T)\nabla\phi) &= 0 && \text{in } \partial\Omega_R\times(0,t_e]\\
\phi &= 0 && \text{in } \partial\Omega_D\times(0,t_e]\\
T(0,x) &= T_0 && \text{on } \Omega\\
T \le T_{max} &\ \text{a.e. in } \Omega\times(0,t_e]\\
0 \le u \le u_{max} &\ \text{a.e. in } (0,t_e]
\end{aligned}$$

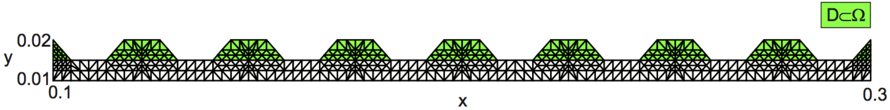
T temperature, ϕ electrical potential, u current

Thermistor Problem with State Constraints

Setup



(a) Domain Ω with boundary Γ_N and Γ_D



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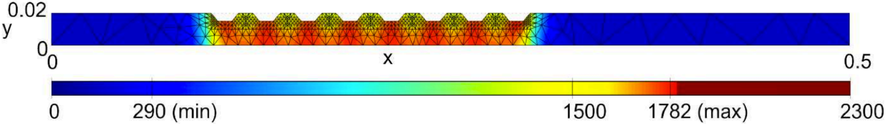
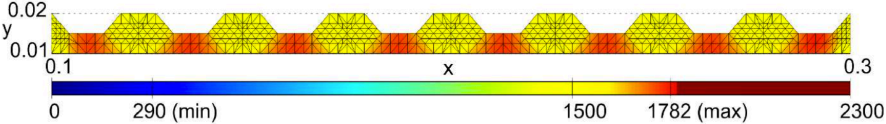
Thermistor Problem with State Constraints

Optimal State (Temperature)



(a) computational domain Ω



(b) subdomain D

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Thermistor Problem with State Constraints

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Iteration History

gamma	no. it.	objective	penalty term	max. pen.	crit. meas.	$\sum$dof	cpt
1.0e+0	0	3.2769e+5	3.2761e+5	9.2458e+2	1.4979e+2	2.37e+4	0.17%
1.0e+1	2	1.2535e+5	1.2534e+4	4.9127e+2	1.2846e+2	2.37e+4	2.66%
1.0e+2	3	1.3885e+4	1.3884e+2	2.4801e+2	3.4204e+1	2.64e+4	4.33%
1.0e+3	2	1.3390e+4	1.3389e+1	1.5877e+2	3.8208e+1	7.24e+4	8.85%
1.0e+4	3	2.5161e+3	2.5155e−1	6.3363e+1	1.5264e+1	6.97e+4	11.45%
1.0e+5	3	2.6217e+2	2.6115e−3	2.4467e+1	3.9273e+0	2.34e+5	44.57%
1.0e+6	2	2.5128e+2	2.5014e−4	1.7350e+1	3.3702e+0	2.32e+5	27.97%

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Conclusions

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- Multilevel optimization with adaptive discretization + ROMs + error estimation promising
- Retardation factor optimization/simulation ≤ 5 seems possible also for time-dependent problems
- Full second order methods applicable, since step is computed on ROM level

Topics for Future Work

- Integration of goal oriented instead of residual based error estimators
- Error estimation for ROMs (with Stefan Volkwein)
- Improvement strategies for ROMs
- ROMs for space-time adaptive discretizations
- Extension to robust optimization (under uncertainty)
- Applications, in particular flow and FSI problems, shape optimization